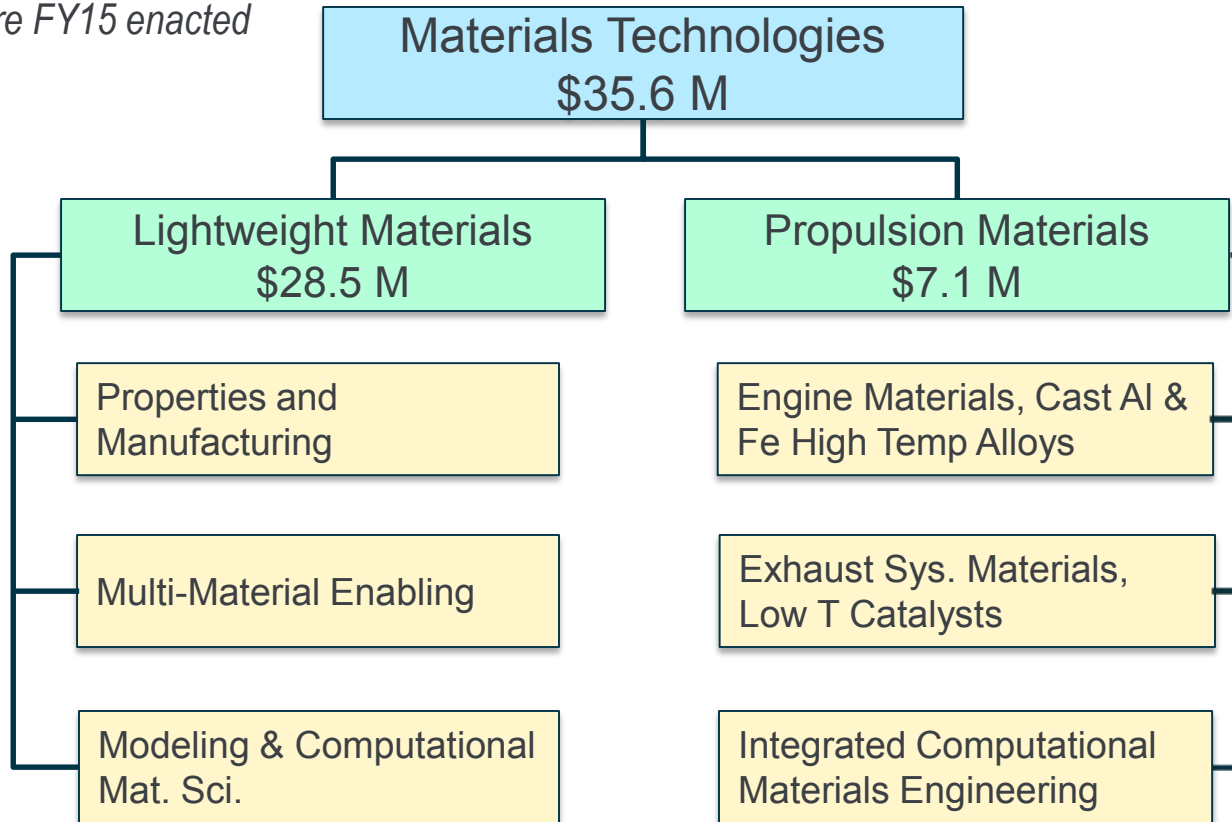




**Vehicle Technologies Office**  
*Propulsion Materials Technologies*

Jerry Gibbs

Values are FY15 enacted



	Lightweight	Propulsion
FY13 Enacted	\$27.5 M	\$11.9 M
FY14 Enacted	\$28.0 M	\$8.9 M
FY15 Enacted	\$28.5 M	\$7.1 M

- Targets powertrain materials requirements for future automotive and heavy-duty applications: engine, transmission, exhaust components, and targeted materials for electric powertrains. As the weight of the vehicle structure is reduced the percentage of the total vehicle weight in the powertrain is increasing.
- Addresses materials for high efficiency Internal Combustion Engines, powertrain materials interactions with new fuel compositions.
- Most (85%) Propulsion Materials projects utilize Integrated Computational Materials Engineering (ICME) to set performance targets and accelerate results in materials discovery, materials formulation, and materials processing techniques.
- Identifies gaps in existing ICME tools and develops new topics to expand the use of computational methods in materials development and materials engineering

# Workshop Propulsion Materials R&D Gaps and Targets

Metric	2013	2050	Material Gaps
Powertrain Weight Reduction (ICE/HEV)	Baseline - LDV Baseline – HDV	40% lighter- LDV 20% lighter- HDV	Structure and Volumetric Efficiency (block, head, transmission; AL ,CF)
Power density	LDVs -2.7L 196 HP (73.4 HP/L)  HD15L 475HP (32 HP/L)	LD 1.3L 196 HP (150 HP/L) LW-LD 0.7L 98 HP  HD 9L 475HP (53 HP/L)	Structure and rotating components (crankshaft, pistons, connecting rods, gears; Steels + )
Energy Recovery	LDV <5% Turbocharged  HD ~99% Turbocharged	LDV ~50% Turbo/ TEs/ Turbo-compounding HD~ 99% Turbo/TEs/ Rankine Cycle/Turbo-compounding	Turbochargers, Superchargers, Turbo-compounding, Rankine Cycle components, seals, fluid interactions
Exhaust Temperatures (Exhaust Valve to Turbo Inlet)	LDV - 800 °C HDV - 700 °C	1000 °C - LDV 900 °C - HDV	Valves (super alloys & Ceramics) E Manifolds, Turbochargers
Cylinder Peak Pressures	LDV ~ 50 bar HDV 190 bar	>103 bar - LDV gasoline >150 bar ATP-DI gasoline >260 bar – HDV	Structure and rotating components , gaskets, valves, friction
Engine Thermal Efficiency	LDV 30% e HDV 42% e	LDV 45% e, Stretch 55+% e HDV 55% e, Stretch 60% e	Control Heat Losses (Pistons, Cylinder wall, Cylinder head, exhaust manifold)

## Light- and Heavy-Duty Roadmaps, US Drive Low T Catalyst Workshop Report

### Engine Materials

#### Improve Engine Efficiency

- Improved Materials
  - Strength
  - Durability
  - Operating T
  - Manufacturability
  - Lower Cost

### Exhaust System Materials

- Low Cost High Temp Alloys for Exhaust Manifolds, Turbocharger Housings and Turbines
- Low Temp Catalyst Materials and ceramic substrates

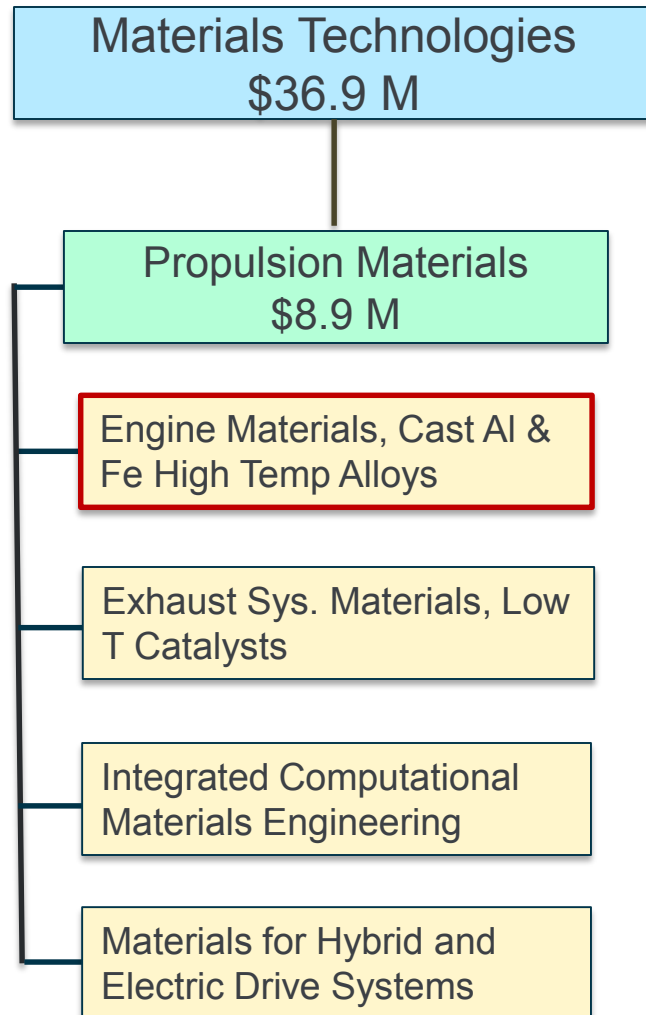
### Integrated Computational Materials Engineering

#### New materials and processes using multi-scale modeling

- Modeling to create tailored materials
- Predict behavior
- Optimizing complex processes

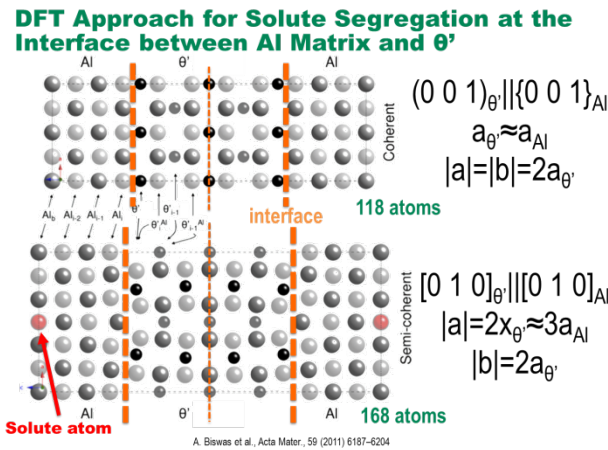
## Demonstration, Validation, and Analysis



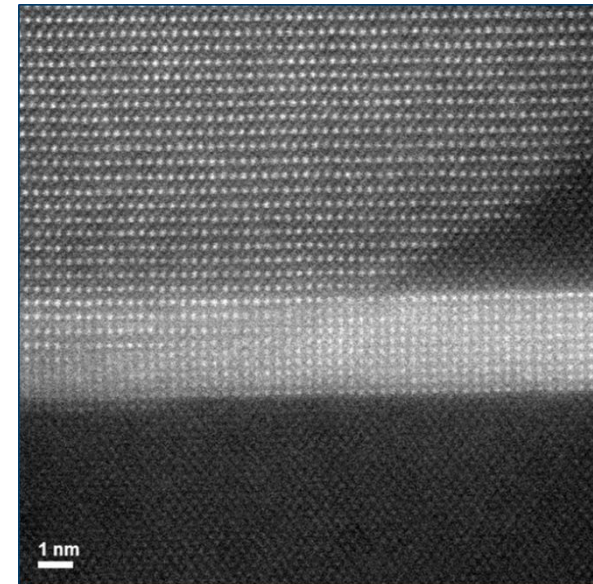
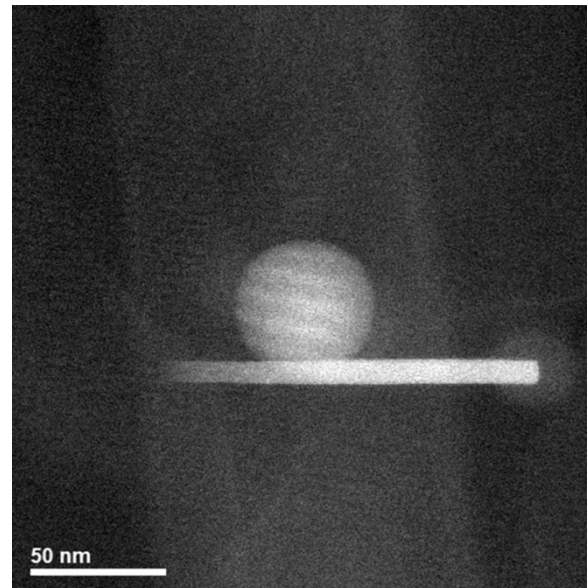
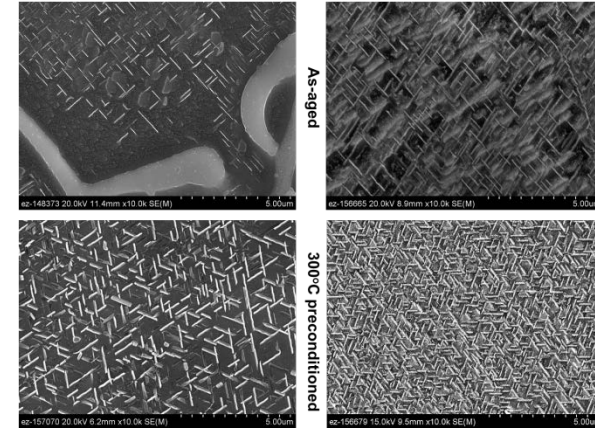


- Targets the Advanced Combustion Engine team stretch goals, 50%+ efficiency for heavy-duty and automotive engines
  - **Lightweight Cast alloys for automotive engines and transmissions:** **GM; Ford; ORNL/Chrysler:** Lightweight high strength aluminum alloy development to replace A356 or A319 and enable higher operating temperatures and higher efficiency combustion regimes.
  - **High performance Cast Ferrous Alloys for Heavy-duty Applications:** **Caterpillar:** High strength, low cost cast alloy development to provide performance superior to Compacted Graphite Iron, easily cast and machined, and at a cost similar to cast iron, enabling engines with higher peak cylinder pressures and increased efficiency.
  - **High performance Cast Steels for Crankshafts:** **Caterpillar/GM:** High performance low cost cast steel providing performance similar to high cost forged steel units, enabling a low cost pathway to increased engine efficiency in automotive and heavy duty applications.

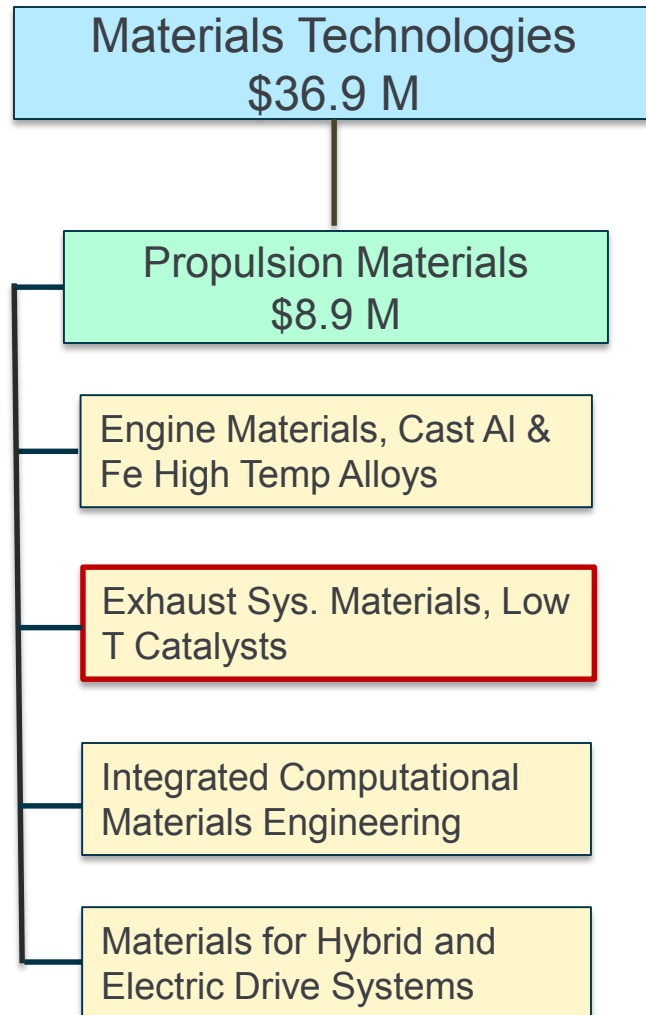
The Propulsion Materials' Cast alloy development program for engine applications combines first principals computational materials design, advanced characterization, and experimental validation resulting in new alloys and expanded ICME capabilities



## Advanced Characterization



# Propulsion Materials– Exhaust System Materials, Low T Catalysts



- Fundamental Catalyst Materials
  - **ORNL**: Evaluation of catalyst microstructures and
- Exhaust Aftertreatment Components
  - **ORNL/Ford**: Impacts of biofuels on component life and development of mitigation strategies
  - **ORNL**: Durability of diesel particulate filters
- Low Temperature Catalyst  
Competitive awards made FY-2014
  - **Ford/ORNL** - Automotive
  - **Chrysler (FCA)/PNNL** - Automotive
  - **Cummins/PNNL** – Heavy-Duty Trucks

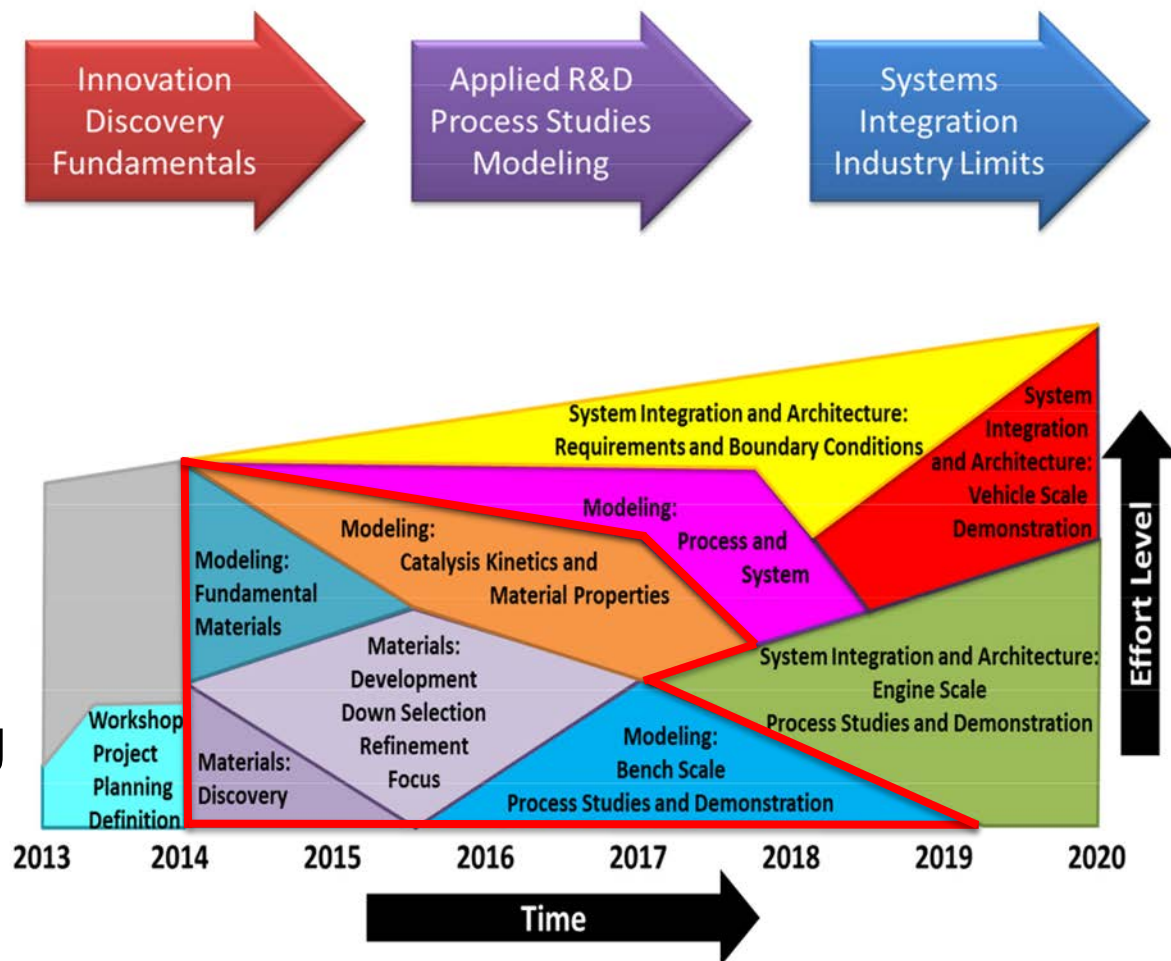


# Propulsion Materials Exhaust System Materials, Low T Catalysts (Cont)

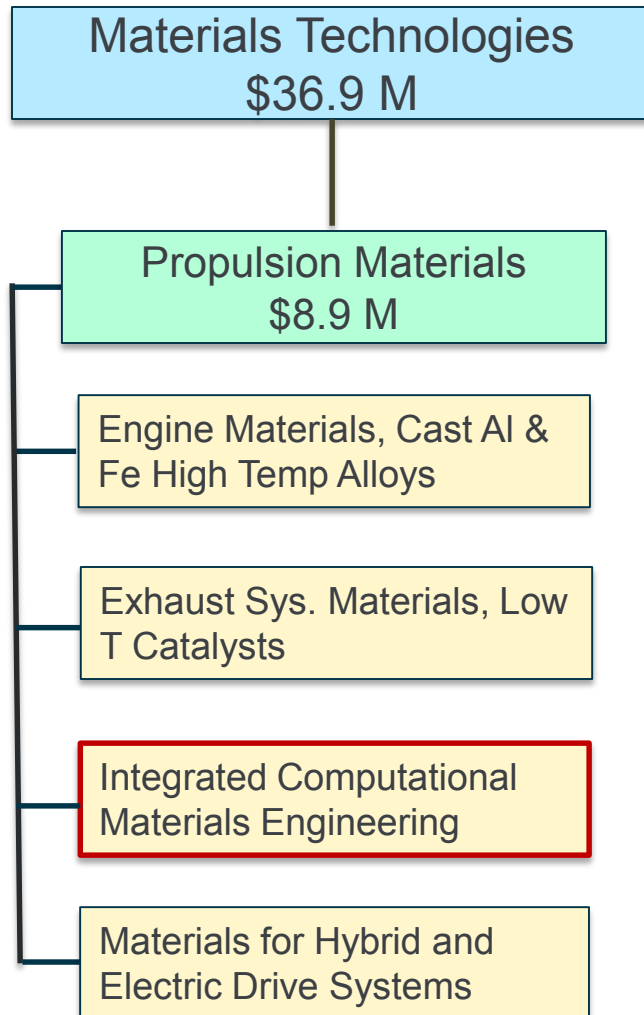
## The Propulsion Materials'

Low Temperature Catalyst development effort is guided by the **US CAR** advanced aftertreatment workshop report and all materials development and validation activities reside in the areas outlined in red bridging materials fundamentals and applied R&D

## Future Automotive Aftertreatment Solutions: The 150°C Challenge Workshop Report



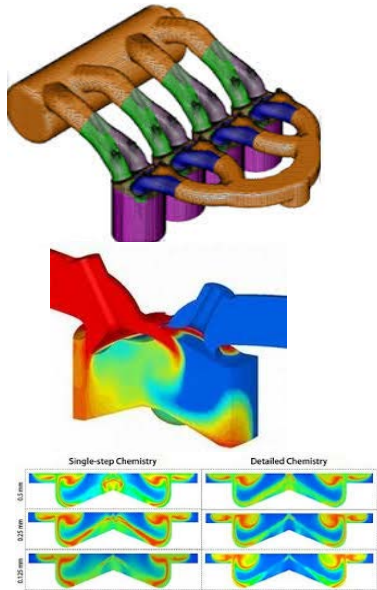
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## – Integrated Computational Materials Engineering

- **ORNL:** Exploratory methods based on First Principles Calculations, Density Functional Theory, and Calculated Density of States to identify new materials compositions with tailored properties:
  - Thermoelectric Materials, 3 new compositions have been validated;
  - Non-rare earth magnetic materials, 2 new compositions have been validated;
  - Low Temperature Catalyst materials, 1 new low temperature catalyst have been validated for Oxides of Nitrogen
- Each Propulsion Materials FOA project includes a multi-scale ICME application, validation, and gap analysis component (two were included in the President's Materials Genome announcement).

## Advanced Combustion Models

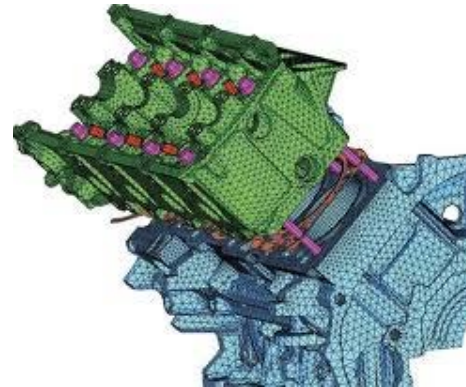


Temperature and pressure  
Boundary conditions



Efficiency  
improvement potential

## Finite Element Baseline Design Constraints

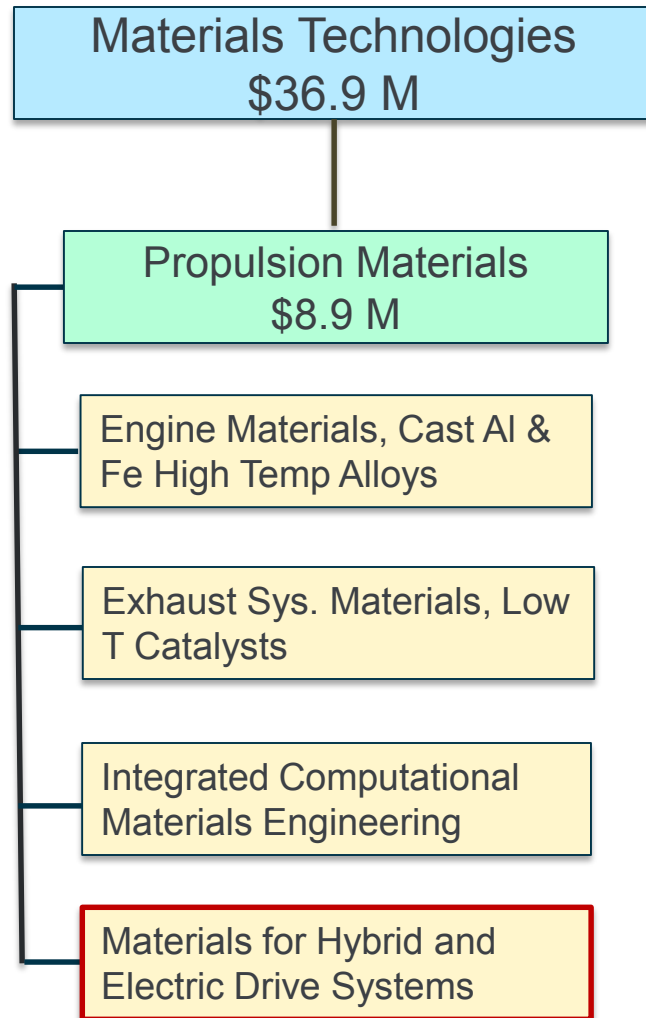


Prioritized  
Components  
and  
Material  
Property  
Targets



**Identify and prioritize the material improvements needed to enable high efficiency combustion systems, and quantify the benefits.**

# Propulsion Materials– Materials for Hybrid and Electric Drive Systems



– Projects very limited in scope to address specific gaps in material properties, materials processing, or material joining

- **ORNL:** Enabling Materials for High Temperature Electronics: Organic materials not 200°C-capable
- **ORNL:** Enabling Materials for High Temperature Electronics: Solders not 200°C-capable
- **PNNL:** Novel Manufacturing Technologies for High Power Induction and Permanent Magnet Electric Motors
- Goal to rapidly transition results to the APEEM team

New non-rare earth magnetic materials are predicted within the ICME activity and validated by the APEEM team



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